THERMODYNAMIC FUNCTIONS OF $TlFeX_2$(X-S, Se, Te) and $TlCrS_2$

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The heat capacity of the $TlFeX_2$(X=S, Se, Te) and $TlCrS_2$ compounds has been measured in the temperature interval 4.2-300 K. The experimental data on the temperature dependence of the heat capacity are used to calculate the thermodynamic parameters of these compounds: the changes in entropy, enthalpy and Gibbs free energy.

Compounds with the general chemical formula $TlMeX_2$ (Me=Co, Ni, Fe, Cr, Mn; X=S, Se,Te) belong to the class of low-dimensional magnets. Results on the synthesis of such compounds and the study of their physical properties are reported in [1-10].

Experimental data on heat capacity and thermodynamic parameters are used in theoretical calculations, in calculations of technological processes, connected with synthesis and growth of compounds. Investigation of thermodynamic characteristics of semiconductors is important in studying of problem of chemical bonds. From the analysis of thermodynamic parameters (entropy, enthalpy, Gibbs free energy) it is possible to obtain the information about chemical bonds in semiconductors. Investigations carried out with the help of method of low-energy calorimetry occupy significant place in complex of works on studying of thermodynamic properties of semiconductors. Thermodynamic functions are calculated the most exactly on the base of calorimetric data.

In present work the heat capacity was measured by an adiabatic method [11]. We investigated the heat capacity of low-dimensional $TlFeX_2$ (X=S, Se, Te) and $TlCrS_2$ magnet semiconductors [12] in the temperature intervals (4.2 -300) K and (60-300)K, correspondingly. It must be noted that below 60 K Cp (T) dependence for $TlCrS_2$ has been extrapolated to$T\rightarrow 0$ by the. Debye low. Thermodynamic characteristics, such as the change in entropy (S_T-S_0), enthalpy (H_T-H_0) and Gibbs free energy (ΔF) have been calculated from temperature dependence of heat capacity in wide temperature range from 0 to 300 K.

The change of entropy, enthalpy and Gibbs free energy have been determined from the following expressions

$$S_T\text{-}S_o=\int_O^T \frac{C_p(T)}{T}dT \qquad (1)$$

$$H_T\text{-}H_o=\int_O^T C_p(T)dT \qquad (2)$$

$$\Delta F=-\left[-\left(S_T-\frac{H_T-H_o}{T}\right)\right] \qquad (3)$$

The values of these thermodynamic characteristics are given in tables 1-4.

Table 1.Evened values of heat capacity and changes in entropy, enthalpy and reduced Gibbs free energy for $TlFeS_2$

T, K	ΔS_T, J/mole·K	ΔH_m, kJ/mole	$-\Delta F_r$, J/mole·K
10	2.87	0.017	1.11
20	11.37	0.146	4.02
50	37.75	1.062	16.49
70	51.46	1.975	23.23
100	71.80	3.703	34.81
120	84.26	5.066	42.02
150	101.1	7.341	52.2
170	111.4	8.97	58.6
200	125.6	11.60	67.6
220	134.3	13.43	73.3
250	146.3	16.25	81.3
270	153.8	18.19	86.4
300	164.2	21.17	93.7

Table 2.Evened values of heat capacity and changes in entropy, enthalpy and reduced Gibbs free energy for $TlFeSe_2$

T, K	ΔS_T, J/K mole	ΔH_T, kJ/mole	$-\Delta F_T$ J/mole K
10	4.22	0.027	1.48
20	14.02	0.176	5.20
50	47.10	1.329	20.52
70	66.59	2.494	30.96
100	91.60	4.609	45.5
120	106.1	6.19	54.4
150	125.1	8.76	66.7
170	136.4	10.56	74.3
200	151.7	13.38	84.7
220	160.9	15.33	91.3
250	173.8	18.34	100.4
270	181.7	20.40	106.1
300	193.5	23.55	114.9

Table 3. Evened values of heat capacity and changes in entropy, enthalpy and reduced Gibbs free energy for $TlFeTe_2$

T, K	ΔS_T, J/K mole	ΔH_m, kJ/mole	$-\Delta F_T$, J/Kmole
10	2.04	0.015	0.52
20	9.90	0.135	3.13
50	40.60	1.219	16.22
70	60.10	2.389	25.97
100	85.9	4.578	40.10
120	101.1	6.241	49.00
150	120.9	8.911	61.5
170	132.6	10.78	69.2
200	148.5	13.71	79.9
220	158.0	15.71	86.6
250	170.9	18.75	95.9
270	178.8	20.81	101.8
300	189.8	23.92	110.1

Table 4.

Evened values of heat capacity and changes in entropy, enthalpy and reduced Gibbs free energy for $TlCrS_2$

T, K	ΔS_T, J/Kmole	ΔH_m, kJ/mole	ΔF_T, J/Kmole
10	5.76	0.024	3.34
20	10.48	0.095	5.78
50	28.50	0.74	13.70
70	42.28	1.568	19.88
100	62.48	3.283	30.10
120	75.30	4.691	36.20
150	93.04	7.081	45.84
170	103.62	8.773	52.02
200	117.86	11.410	60.76
220	126.56	13.230	66.46
250	138.42	16.012	74.37
270	145.66	17.898	79.37
300	155.74	20.766	86.52

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$TlFeX_2$(X-S, Se, Te) və $TlCrS_2$ TERMODİNAMİK FUNKSİYALARI

$TlFeX_2$ (X=S, Se, Te) və $TlCrS_2$ birləşmələrinin 4,2-300 K intervalında istilik tutumu ölçülmüşdür. İstilik tutumunun eksperimental olaraq temperatur asıllığından alınmış qiymətlərindən göstərilən birləşmələrinin termodinamik parametrlərinin hesablanmasında istifadə edilmişdir: entropiyanın, entalpiyanın və Qibsin sərbəst enerjisinin dəyişməsi.

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ТЕРМОДИНАМИЧЕСКИЕ ФУНКЦИИ $TlFeX_2$(X-S, Se, Te) и $TlCrS_2$

В широком температурном интервале 4.2-300K измерена теплоемкость соединений $TlFeX_2$ (X=S, Se, Te) и $TlCrS_2$. Экспериментальные результаты по изучению температурной зависимости теплоемкости использованы для вычисления термодинамических параметров указанных соединений: изменение энтропии, энтальпии и свободной энергии Гиббса.

Received: 20.05.09